Philippe P. Pébay

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February 28, 2005

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1 Education and Degrees

Qualification aux Fonctions de Maître de Conférences, 2003
Section: 26$^{\text{th}}$, Applied Mathematics and Applications of Mathematics
Awarded by the French National Council of Universities
Certification that grants the permissision to apply for associate professor (*Maître de Conférences*) positions at French universities.

PhD (*Doctorat*) **in Mathematics**, University of Paris-6, 2000
Specialty: Analyse Numérique
Title: *A priori* Delaunay-conformity in 2 and 3 dimensions.
Jury:

O. Pironneau	Académie des Sciences & Professeur, Paris-6	Chair
T.J. Baker	Senior Research Scientist, Princeton University	Reviewer
J.D. Boissonnat	Directeur de Recherches, INRIA Sophia	Reviewer
F. Hecht	Professeur, University of Paris-6	Advisor
P.L. George	Directeur de Recherches, INRIA Rocquencourt	Co-advisor
J. Pousin	Professeur, INSA Lyon	Examiner

Agrégation **in Mathematics**, 1994
Option: Probabilities
French nationwide competitive graduate selection

MS (*Diplôme d'Études Approfondies*) **in Computer Science**, University of Strasbourg-1, 1992

BS (*Maîtrise*) **in Mathematics**, University of Strasbourg-1, 1991
BS (*Maîtrise*) **in Mathematical Engineering**, University of Strasbourg-1, 1991

2 Research

2.1 Summary

My research activity pertains to the fields of **applied mathematics and scientifig computing**.

My first specialty is that of mesh generation and adaptation. Essential to numerous applications, it is however a young subject. Despite the fact that several different types of methods have appeared and have been implemented within a few years, numerous problems remain open. For example,

while a method that constructs a Delaunay triangulation displays indisputable advantages in terms of robustness and speed,it is intrisically unable to take into account topological constraints, even only domain nonconvexity. That constitutes a serious obstacle to using such methods in applications. Another class of open questions is that of mesh improvement and adaptation; in particular, prior to adapting a mesh to a given problem, one must first wonder how to answer to the question *what is a good mesh?*
My efforts in mesh generation and adaptation have been conducted mostly in these two directions: on the one hand, in the context of my PhD research work with P.-L. George (INRIA) and F. Hecht (Paris-6), on Delaunay simplicial mesh generation for arbitrary geometires, by the means of the theory and algorithms I have and called "*a priori* Delaunay-redefinition"; on the other hand, during my post-doctoral work with T. Baker (Princeton) as well as for part of my time at Sandia National Laboratories, on the quality assessment and adaptation of meshes. In particular, I am developing novel parallel mesh refinement methods, in the context of the scientific visualization toolkit `VTK` and of the parallel visualization appllication `ParaView`.

My research activity in other fields than meshing and its applications began when I joined Sandia National Laboratories. One of these new subjects is motivated by uncertainty quantification in fluid mechanics and chemistry, in particular in combustion, by the means of stochastic methods. With the group lead by H. Najm (Sandia), in collaboration with O. Knio (J. Hopkins) and O. Le Maître (U. Évry), we are designing, implementing and validating intrusive stochastic methods based on Hermite-Gauss polynomial chaoses (Wiener spaces). This work on novel numerical methods (*e.g.*, publication in the *SIAM J. on Scientific Computing*), has already brought new insights into combustion processes, (*e.g.*, publication in the *Int. J. on Chemical Kinetics*).

Due to the applied engineering mission of Sandia National Laboratories, I also came to work with other applications of mathematics to scientific computing, such as the development and implementation of numerical methods for parallel computational combustion codes – as well as the optimization of existing methods. For instance, the development of a higher order time-integrator for low Mach number reacting flows, that is suitable for both parallelization and automatic adapation of semistructured meshes (AMR). In this goal, I have conducted my research in two directions: on the one hand, half-explicit schemes for differential-algebraic equations with index 2 (DAE2); on the other hand, variational formulation of constrained PDEs. Theoretical results have been published, and development is in progress. Indeed, a substantial part of my work focuses mon the actual reality of scientific computing, *i.e.*, programing, porting, debuging, testing and optimizing codes and/or libraries on different platforms, and following the evolution of compilers, architectures, and languages.

2.2 Outline

Sandia National Laboratories, U.S.A.
Technical Staff, since April 2002
I have been recruited by Sandia's *Computational Modeling and Simulation of Reacting Flows* and *High Performance Computing and Networking* to contribute in the research and development of massively parallel codes, in particular for computational combustion, and of toolkits for the visualization and analysis of large scale numerical simulations. My work can be summarized in applied mathematics for scientific computing. More precisely, my research fields are:

- design and development of algorithm for the visualization and analysis of 3D higher order finite elements simulations; in particular, design and implementation of new tools in `VTK` and `ParaView` [1, 2, 22, 23];
- development of new schemes for constrained ODEs and PDEs, such as those met in the low Mach number approximation [5, 11, 24, 26, 35, 36];
- assessment of mesh quality and mesh adaptation [6, 34, 12, 19, 20];
- uncertainty quantification with stochastic methods [3, 4, 18];

- programing and optimizing these methods and alforithms in `C/C++`, `Fortran` and `MPI`;
- porting and evaluating parallel codes for numerical combustion to `Linux` clusters with several hundereds of CPUs ((Intel ou AMD) and Infiniband backbones.

Projet Gamma, INRIA Rocquencourt, France
Consultant, 2002 (4 mnoths)
In collaboration with P. Frey, modification of `Medit`, INRIA's mesh and numerical solutions visualization code, for MSC Software, world leader in simulation software(`Nastran`, `Patran`, `Marc`, *etc.*). Developement in `C/C++` et `OpenGL`.

Mechanical and Aerospace Engineering Department, Princeton University, U.S.A.
Visiting Research Staff, 2001
Post-doctoral appointment in Pr L. Martinelli's group, under the guidance of T.J. Baker, with whom I worked on the development of his dynamic tetrahedral mesher. In particular, this has brought us to the study of the notion of mesh quality [7, 14, 27]. In addition, collaboration with the CREATIS laboratory of INSA Lyon, France, for the application of dynamic meshing to human heart simulation [13, 37].

INRIA Rocquencourt and INSA Lyon, France
PhD fellow at INRIA, 1996–2000 and *Professeur Agrégé* (tenured lecturer) at INSA, 1997-2000
In the context of my PhD research work [38], conducted under the guidance of P.L. George, design for the *a priori* Delaunay-conforming redefinition of 2D et 3D constraints, allowing exact Delaunay mesh generation of arbitrary domains [8, 15, 16, 28, 29]. The algorithms I proposed and implemented have been validated by successfully meshing domains for which `GHS3D`, INRIA's tetrahedral mesher, was not converging.

Biomedial Thermology Laboratory, Strasbourg School of Medicine, France
Research and Teaching Assistant, 1992–1994
The laboratory was working with Val-de-Grâce hospital in Paris and Thomson-CGR on treatment planning of ultrasonic thermotherapy of brain tumours. I was working with P. Frey (then a graduate student, now a Professor at the University of Paris-6) to develop a thermo-acoustic finite element solver [17]. However, General Electric bought CGR and the research grant stopped; this is why I decided to pass the *Agrégation*, so that I could prepare a PhD degree with my own support.

CNRS-LSIIT, Strasbourg, France
Graduate Intern, 1992 (6 months)
Design of an algorithm for the deformation of 3D objects with constant volume. Implementation (`C`) as extensions to the `DOGME` code (IBM / Pr D. Bechmann) [39].

Dassault Aviation, Directorate for Advanced Studies, Saint-Cloud, France
Undergraduate Intern, 1991 (3 months)
Characterization of the mathematical limitations of numerical simulation (with L. Zimmer). Implementation (`Prolog`) of enhancements to the qualitative simulator `QSIM`.

3 Teaching

3.1 Summary

Since 1992, I have taught more than 1000 hours of mathematics at higher education institutions. Most of my teaching activity took place at undergraduate departments of INSA Lyon (National Institute for Applied Sciences), France's largest school of engineering and applied sciences, covering the majority of the mathematical topics classically taught at this level. More specifically, a colleague

and myself have designed and implemented the mathematical curriculum for the ASINSA department, created in 1999 at INSA Lyon. Dedicated to students from Asian countries, and for students learning at least one asian language, this curriculum had to be specific due to the very diverse educational backgrounds of the students (half a dozen Asian countries). I also taught the numerical analysis class of the newly created "Bioinformatics and Modelization" department in 2000.
At graduate and postgraduate level, I taught automatic mesh generation at INSA (Master's degree program), and an introduction to measure theory and its applications to stochastic methods at Sandia National Laboratories (with lectures notes [25]).

3.2 Outline

Sandia National Laboratories, U.S.A.
Lectures (40 hours) in the spring of 2003, on measure theory and its applications to stochastic methods, for a group of researchers in numerical combustion and applied mathematics.

INSA Lyon, France
Professeur Agrégé (tenured lecturer), Mathematics, 1997 – 2000
Undergraduate lectures and precepts in analysis and introduction to topology, general algebra, linear and bilinear algebra, differential and integral calculus, geometry and applications, numerical analysis.
Graduate lectures on mesh generation.

Institute for Teaching Training, University of Bordeaux, France
Following *Agrégation* nationwide selection, training prior to tenure with the French Department of Education (includes a high school assignment).

School of Sciences, University of Strasbourg-1, France
Teaching Assistant, 1992–94
Precepts in mathematics for undergraduate students: analysis, algebra, modelization and differential equations.

4 Other Professional Activities

4.1 Organization

Committee member of the 14$^{\text{th}}$ **International Meshing Roundtable**, 2005
`www.imr.sandia.gov`

Organizer of the **Mini-Symposium on Numerical Simulation of Low Mach Number Flows**
SciCADE03, Trondheim, Norway, June 30 – July 4 2003
`www.math.ntnu.no/scicade/talks.php?msid=1930902167`

Organizer of the **Workshop on Mesh Quality and Dynamic Meshing**
Sandia National Laboratories, Livermore, U.S.A., January 16 & 17 2003
`www.ca.sandia.gov/CRF/mqdm`

4.2 Review

Reviewer for:

- International Journal of Computing and Information Science in Engineering
- Journal of Computational Physics
- 13$^{\text{th}}$ International Meshing Roundtable
- 11$^{\text{th}}$ International Meshing Roundtable

4.3 System Administration

Mechanical and Aerospace Engineering Department, Princeton University, U.S.A.
Installation and system administration of a 32-CPU textttLinux cluster with Myrinet 2k backbone.

INSA Lyon, France
System administration and hardware maintenance of the computer systems of the Center for Mathematics, 1999–2000 (*ca.* 30 `Linux` PCs and `X` terminals).

5 References

Articles in Refereed Journals

Published or Accepted

[1] D. C. Thompson and P. P. Pébay. Embarassingly parallel mesh refinement. *Engineering with Computers*. Invited January 2005.

[2] P. P. Pébay and D C. Thompson. Communication-free streaming mesh refinement. *ASME Transactions, Journal of Computing & Information Science in Engineering, Special Issue on Mesh-Based Geometry*, 2005. In print.

[3] M. T. Reagan, H.N. Najm, P. P. Pébay, O. M. Knio, and R. G. Ghanem. Quantifying uncertainty in chemical systems modeling. *International Journal of Chemical Kinetics*, 36, 2005. In print.

[4] B. J. Debusschere, H.N. Najm, P. P. Pébay, O. Knio, R.G. Ghanem, and O. P. Le Maître. Numerical challenges in using polynomial chaos. *SIAM J. Scientific Computing, Special Issue on Uncertainty Quantification*, 26(2):698–719, 2004.
`dx.doi.org/10.1137/S1064827503427741`.

[5] P. P. Pébay, H. N. Najm, and J. G. Pousin. A non-split projection strategy for low Mach number flows. *Int. J. for Multiscale Computational Engineering*, 2(3):445–460, 2004.
`dx.doi.org/10.1615/IntJMultCompEng.v2.i3.60`.

[6] P. P. Pébay. Planar quadrangle quality measures. *Engineering with Computers*, 20(2):157–173, 2004.
`dx.doi.org/10.1007/s00366-004-0280-8`. Invited.

[7] P. P. Pébay and T. J. Baker. Analysis of triangle quality measures. *Mathematics of Computation*, 72(244):1817–1839, 2003.
`dx.doi.org/10.1090/S0025-5718-03-01485-6`.

[8] P. P. Pébay and P. J. Frey. Delaunay-conformity of surface triangulations. *C.R. Acad. Sci. Paris, Sér. I Math.*, 327(3):313–318, 1998.
`dx.doi.org/10.1016/S0764-4442(98)80152-3`.

Submitted

[9] E. R. Hawkes, R. Sankaran, P. P. Pébay, and J. H. Chen. Direct numerical simulation of ignition front propagation in a constant volume with temperature inhomogeneities. Part II: Parametric study. *Combustion and Flame*. Submitted December 2004.

Articles in Refereed International Conferences Proceedings

[10] P. P. Pébay and D. C. Thompson. Parallel mesh refinement without communication. In *Proc. 13th International Meshing Roundtable*, pages 437–448. Williamsburg, VA, September 2004. `http://www.andrew.cmu.edu/user/sowen/abstracts/Pe1031.html`.

[11] J. G. Pousin, P. P. Pébay, M. Picq, and H. N. Najm. Solving the transport equation subject to an affine constraint. In *Proc. ECCOMAS 2004*. Jyväskylä, Finland, July 2004. `www.mit.jyu.fi/eccomas2004/proceedings/pdf/182.pdf`.

[12] P. P. Pébay. Planar quadrangle quality measures: is there really a choice? In *Proc. 11th International Meshing Roundtable*, pages 53–62. Ithaca, NY, September 2002. `www.andrew.cmu.edu/user/sowen/abstracts/Pe849.html`.

[13] P. P. Pébay, J. G. Pousin, and T.J. Baker. Dynamic meshing for finite element based segmentation of cardiac imagery. In *Proc. 5th World Cong. on Computational Mechanics*. Vienna, Austria, July 2002. `wccm.tuwien.ac.at/cgi-bin/wccm/showDB.pl?showSession&id=M157`. Accepted, not presented.

[14] P. P. Pébay and T. J. Baker. A comparison of triangle quality measures. In *Proc. 10$^{\text{th}}$ International Meshing Roundtable*, pages 327–340. Newport Beach, CA, October 2001. `www.andrew.cmu.edu/user/sowen/abstracts/Pe838.html`.

[15] P. P. Pébay. A new approach towards delaunay-conformity in 3 dimensions. In *Proc. 9$^{\text{th}}$ International Meshing Roundtable*, pages 283–292. New Orléans, LA, October 2000. `www.andrew.cmu.edu/user/sowen/abstracts/P\%E9753.html`.

[16] P. P. Pébay and P. J. Frey. A priori delaunay-conformity. In *Proc. 7$^{\text{th}}$ International Meshing Roundtable*, pages 321–333. Dearborn, MI, October 1998. `www.andrew.cmu.edu/user/sowen/abstracts/Pe593.html`.

[17] P. P. Pébay. Automatic 3d mesh generator based upon mri voxel data for 3d numerical acoustic and thermal modeling using the finite element method. In *Proc.* 2$^{\text{nd}}$ *European Conf. on Engineering and Medicine*. Stuttgart, April 1993.

Articles in Non-Refereed Conferences Proceedings

[18] M. T. Reagan, H. N. Najm, P. P. Pébay, O. M. Knio, and R. G. Ghanem. Uncertainty quantification in reacting flow modeling. In *Western States Section of the Combustion Institute 2004 Spring Meeting*. WSS/CI, UC Davis, CA, March 2004.

[19] H. N. Najm, J. Ray, , C. Kennedy, R. McCoy, S. Lefantzi, P. P. Pébay, and W. Kollmann. Low Mach number reacting flow modeling with structured adaptive mesh refinement. In *Proc. Workshop on Mesh Quality and Dynamic Meshing*, pages 91–106. Sandia National Laboratories, Livermore, CA, January 2003. `www.ca.sandia.gov/CRF/mqdm/pdfs/mqdmproceedings.pdf`.

[20] P. P. Pébay. New results on quality measures for planar quadrilateral meshes. In *Proc. Workshop on Mesh Quality and Dynamic Meshing*, pages 107–138. Sandia National Laboratories, Livermore, CA, January 2003. `www.ca.sandia.gov/CRF/mqdm/pdfs/mqdmproceedings.pdf`.

Technical Reports

[21] P. P. Pébay. The SANDmath package. Sandia Report SAND2004-3894, Sandia National Laboratories, August 2004.
`www.cs.sandia.gov/~rolf/SANDreport/SAND2004-3894.pdf`.

[22] D. C. Thompson and P. P. Pébay. Performance of a streaming mesh refinement algorithm. Sandia Report SAND2004-3858, Sandia National Laboratories, August 2004.
`infoserve.sandia.gov/sand_doc/2004/043858.pdf`.

[23] D. C. Thompson, R. Crawford, R. Khardekar, and P. P. Pébay. Visualization of higher order finite elements. Sandia Report SAND2004-1617, Sandia National Laboratories, April 2004.
`infoserve.sandia.gov/sand_doc/2004/041617.pdf`.

[24] J. G. Pousin, P. P. Pébay, M. Picq, and H. N. Najm. A variational solution to the transport equation subject to an affine constraint. Sandia Report SAND2004-8096, Sandia National Laboratories, February 2004.
`infoserve.sandia.gov/sand_doc/2004/048096.pdf`.

[25] P. P. Pébay. A short course on measure and probability theories. Sandia Report SAND2004-8095, Sandia National Laboratories, February 2004.
`infoserve.sandia.gov/sand_doc/2004/048095.pdf`.

[26] P. P. Pébay, H. N. Najm, and J. G. Pousin. A half-explicit, non-split projection method for low Mach number flows. Sandia Report SAND2004-8080, Sandia National Laboratories, February 2004.
`infoserve.sandia.gov/sand_doc/2004/048080.pdf`.

[27] P. P. Pébay. Some results about the quality of planar mesh elements. Research Report RR-4436, INRIA, April 2002.
`www.inria.fr/rrrt/rr-4436.html`.

[28] P. P. Pébay. Construction d'une contrainte Delaunay-admissible en dimension 2. Research Report RR-3492, INRIA, September 1998.
`www.inria.fr/rrrt/rr-3492.html`.

[29] P. P. Pébay. Construction d'une triangulation surfacique Delaunay-admissible. Research Report RR-3369, INRIA, March 1998.
`www.inria.fr/rrrt/rr-3369.html`.

Other Communications

Posters

[30] D. C. Thompson and P. P. Pébay. Communicationless parallel mesh refinement. In *13th International Meshing Roundtable Poster Session*. Williamsburg, VA, September 2004.
`www.imr.sandia.gov/13imr/sessions.html`.

[31] J. H. Chen, P. P. Pébay, M. W. Sukalski, E. Hawkes, H. Im, and R. Sankaran. Direct numerical simulation of ignition on Catalyst using LA-MPI. In *ClusterWorld Conference & Expo*. San Jose, CA, April 2004.
`www.clusterworldexpo.com`.

Abstracts

[32] P. P. Pébay and D. C. Thompson. Optimizing tetrahedral quality during streaming mesh refinement. In *SIAM Conf. Computational Science and Engineering*. Orlando, FL, February 2005. Abstract.

[33] P. P. Pébay, J. H. Chen, H. Chen, and E. Hawkes. Direct numerical simulation for homogeneous charge compression auto-ignition using scalable parallel I/O. In *SC2004 High Performance Computing, Networking and Storage Conference*. Pittsburgh, PA, November 2004.
`www.vtksolutions.com/StorCloud/apps/app9.shtml`. Abstract and live demonstration.

[34] P. T. Boggs, P. Howard, K. R. Long, S. Margolis, and P. P. Pébay. Rapid source-inversion for chemical/biological attacks. In 11$^{\text{th}}$ *SIAM Conf. Parallel Processing for Scientific Computing*. SIAM, San Francisco, CA, February 2004.
`www.siam.org/confpart/sess/dsp_programsess.cfm?SESSIONCODE=3095`. Abstract.

[35] P. P. Pébay. Half-explicit methods: the new generation of low Mach number time-integrators? NTNU, Trondheim, Norway, July 2003.
`www.math.ntnu.no/scicade/slides/pebay.pdf`. Abstract and slides.

[36] P. P. Pébay. Half-explicit Runge-Kutta scheme for low Mach number reacting flows. In *Workshop on Innovative Time Integrators for PDEs*. CWI, Amsterdam, Netherlands, November 2002.
`www.cwi.nl/events/2002/IIPDE/abstdata/PhilippePPebay/pebay.ps`. Abstract.

[37] P. P. Pébay. 3d moving meshes. In *Journée Imagerie et Maillages Déformables*. INSA Lyon, Villeurbanne, France, June 2002.
`maths.insa-lyon.fr/Actualites/020610.html`. Abstract.

Theses

[38] P. P. Pébay. *Delaunay-conformity in* 2 *and* 3 *dimensions*. PhD in Mathematics thesis (in French), Université Pierre et Marie Curie, Paris-VI, June 2000.
`www.inria.fr/rrrt/tu-0638.html`.

[39] P. P. Pébay. *Déformation d'objets à volume constant*. MS in Computer Science thesis (in French), Université Louis Pasteur, Strasbourg-I, September 1992.